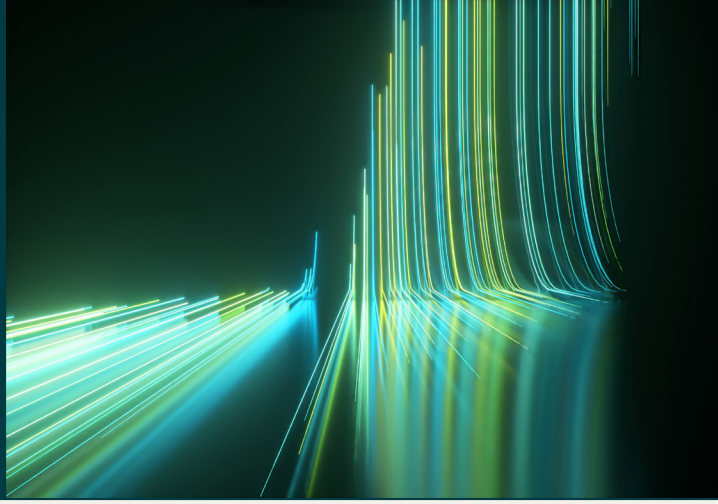
WILEY

Spectral Databases

From the leader in spectral data



Raman - Computed Library of General Compounds - Wiley

Spectra – 196

This database is only available as part of the KnowItAll Raman Spectral Library subscription.

Description

Raman spectroscopy provides materials scientists with a reliable way to identify and characterize inorganic compounds through their unique molecular fingerprints. This is a computed (theoretical) Raman database: spectra were calculated using accurate hybrid functionals rather than obtained through physical measurement.

The database enables researchers to compare experimental and theoretical Raman spectra, investigate vibrational properties, and gain deeper insights into molecular structure and chemical composition. It is particularly useful for materials science, chemistry, spectroscopy research, and educational applications where computational spectral references complement experimental measurements.

By providing reliable theoretical Raman spectra across a broad range of compounds, the database serves as a valuable resource for scientists, researchers, and analysts involved in compound characterization, spectral assignment, and computational spectroscopy studies.

Applications

- Compound identification and characterization
- Computational chemistry and spectroscopy research
- Materials science research
- Experimental-theoretical spectral comparison
- Educational and reference applications

Additional information

When it comes to spectral analysis, the more data you have the better. Wiley spectral databases provide much more information than simply the spectrum. Database records include the following valuable details when available:

- Chemical structure
- Chemical name
- Formula
- InChI/InChIKey
- Molecular weight

Compound coverage

- Computationally generated Raman spectra
- Inorganic compounds
- General chemical compounds
- Molecular and crystalline materials
- Research and reference compounds
- Theoretical spectroscopy datasets

Compatibility

- Subscription includes KnowItAll ID Expert software for one-click basic spectral searches
- Optional: KnowItAll Analytical Edition (recommended for advanced analysis)
- Import spectra from most Raman instruments for direct comparison to reference spectra. For instrument compatibility, visit sciencesolutions.wiley.com/compatibility.

Trusted data from a trusted source

Wiley is the authoritative source for spectral data. Our renowned databases are processed according to rigorous protocols to ensure they are of the highest quality. Qualification procedures start at data acquisition and continue throughout the database development process. Any data acquired from trusted partners is thoroughly vetted before inclusion in our collections.